

A. Supplementary Material

In this section we present proofs of the various theorems in the paper. Recall that given a dataset X and its representation by a hierarchical tree, Eq. (5) defined a tree metric $d(x, y)$, whereas Eq. (6) defined (C, α) -Hölder smooth functions with respect to the tree metric. Let $f : X \rightarrow \mathbb{R}$. For any subset $Y \subset X$ we denote the mean and variance of f on Y as follows,

$$m(f, Y) = \frac{1}{|Y|} \sum_{x \in Y} f(x) \quad (16)$$

$$\sigma^2(f, Y) = \frac{1}{|Y|} \sum_{x \in Y} (f(x) - m(f, Y))^2. \quad (17)$$

Next, given the tree metric we denote by $B(x, r)$ the ball of radius r around x , that is

$$B(x, r) = \{y \in X \mid d(x, y) \leq r\}$$

Observe that by definition, these balls are exactly the different folders of the tree that contain the node x .

The following lemma, standard in the theory of spaces of homogeneous type, will be useful in our proofs.

Lemma 1 *For any $x \in X$, $s > 0$ and $r > 0$ we have*

$$\int_{B(x, r)} d(x, y)^s d\nu(y) = \frac{1}{|X|} \sum_{y \in B(x, r)} d(x, y)^s \leq C_s r^{s+1} \quad (18)$$

with $C_s = 2^{s+1} \left(1 - \frac{1}{2} \underline{B}\right) \leq 2^{s+1}$.

Proof: Recall that by the definition of the tree metric, $d(x, y) \leq 1$, for any $x, y \in X$. Let $K \in \mathbb{N}$ be such that $2^{-K-1} < r \leq 2^{-K}$. Then

$$B(x, r) \subset \biguplus_{k=K}^{\infty} \left[B(x, 2^{-k}) \setminus B(x, 2^{-(k+1)}) \right]$$

Hence

$$\begin{aligned} \int_{B(x, r)} d(x, y)^s d\nu(y) &\leq \sum_{k=K}^{\infty} \int_{B(x, 2^{-k}) \setminus B(x, 2^{-(k+1)})} d(x, y)^s d\nu(y) \\ &\leq \sum_{k=K}^{\infty} \int_{B(x, 2^{-k}) \setminus B(x, 2^{-(k+1)})} 2^{-ks} d\nu(y) \\ &\leq \sum_{k=K}^{\infty} 2^{-ks} \cdot \nu \left(B(x, 2^{-k}) \setminus B(x, 2^{-(k+1)}) \right) \\ &\leq \sum_{k=K}^{\infty} \left[2^{-ks} \left(2^{-k} - \underline{B} \cdot 2^{-(k+1)} \right) \right], \end{aligned}$$

where the last inequality follows from the tree balance condition, Eq. (2). This gives

$$\begin{aligned} \int_{B(x, r)} d(x, y)^s d\nu(y) &\leq \left(1 - \frac{1}{2} \cdot \underline{B} \right) \cdot \sum_{k=K}^{\infty} \left(\frac{1}{2^{s+1}} \right)^k \\ &\leq 2^{s+1} \left(1 - \frac{1}{2} \cdot \underline{B} \right) (2^{-K})^{s+1} \leq 2^{s+1} \left(1 - \frac{1}{2} \cdot \underline{B} \right) r^{s+1}. \end{aligned}$$

□.

Before proving theorem 1, we first introduce an alternative definition of function smoothness:

Definition A.1 A function $f : X \rightarrow \mathbb{R}$ is (C, α) -Mean Hölder (w.r.t. the tree metric d) if for all $x \in X$ and any ball $B(x, r)$,

$$\sigma(f, B(x, r)) \leq C \cdot \nu(B(x, r))^\alpha. \quad (19)$$

where $\sigma(f, B(x, r))$ is defined in Eq. (17).

The following lemma shows that the two definitions of function smoothness w.r.t. the tree metric are related.

Lemma 2 Let $f : X \rightarrow \mathbb{R}$ be (C, α) -Hölder with respect to the tree. Then f is $(2^{\alpha+1}C, \alpha)$ mean-Hölder.

Proof of Lemma: Let $x \in X$ and let B be any ball around x . Since X is finite, for any $\varepsilon \geq 0$ small enough, we have $B = B(x, r)$ for $r = \nu(B) + \varepsilon$. Now,

$$\begin{aligned} \int_B (f(x) - m(f, B))^2 d\nu(x) &= \int_B \left(f(x) - \frac{1}{\nu(B)} \int_B f(y) d\nu(y) \right)^2 d\nu(x) \\ &= \frac{1}{\nu^2(B)} \int_B \left(\int_B f(x) - f(y) d\nu(y) \right)^2 d\nu(x) \leq \\ &\leq \frac{1}{\nu^2(B)} \int_B \left(\int_B |f(x) - f(y)| d\nu(y) \right)^2 d\nu(x). \end{aligned}$$

As $f : X \rightarrow \mathbb{R}$ is (C, α) -Hölder, this gives

$$\int_B (f(x) - m(f, B))^2 d\nu(x) \leq \left(\frac{C}{\nu(B)} \right)^2 \int_B \left(\int_B d(x, y)^\alpha d\nu(y) \right)^2 d\nu(x).$$

We now substitute $s = \alpha$ in Lemma 1 to obtain

$$\begin{aligned} \int_B (f(x) - m(f, B))^2 d\nu(x) &\leq \left(\frac{C}{\nu(B)} \right)^2 \int_B (2^{\alpha+1} r^{\alpha+1})^2 d\nu(x) \\ &\leq \left(\frac{2^{\alpha+1} C}{\nu(B)} \right)^2 \nu(B) r^{2\alpha+2} \\ &\leq \left(\frac{2^{\alpha+1} C}{\nu(B)} \right)^2 \nu(B) (\nu(B) + \varepsilon)^{2\alpha+2}. \end{aligned}$$

Since ε can be arbitrarily small, we conclude that

$$\int_B (f(x) - m(f, B))^2 d\nu(x) \leq \left(\frac{2^{\alpha+1} C}{\nu(B)} \right)^2 \nu(B)^{2\alpha+3} = (2^{\alpha+1} C)^2 \nu(B)^{2\alpha+1}$$

and therefore

$$\sigma(f, B) = \sqrt{\frac{1}{\nu(B)} \int_B (f(x) - m(f, B))^2 \nu(x)} \leq C 2^{\alpha+1} \nu(B)^{\alpha+1/2}. \quad (20)$$

Since $\nu(B) \leq 1$, the theorem follows. \square .

Proof of Theorem 1: Recall that by definition, each Haar-like basis function $\psi_{\ell, k, j}$ is supported on the folder X_k^ℓ . It also has zero mean, namely $\int_{X_k^\ell} \psi_{\ell, k, j}(x) d\nu(x) = 0$, and unit norm, namely $\int_{X_k^\ell} \psi_{\ell, k, j}^2(x) d\nu(x) = 1$. Therefore,

$$\langle f, \psi_{\ell, k, j} \rangle = \int_{X_k^\ell} f(x) \psi_{\ell, k, j}(x) d\nu(x) = \int_{X_k^\ell} (f(x) - m(f, X_k^\ell)) \psi_{\ell, k, j}(x) d\nu(x).$$

The Cauchy–Schwartz inequality now yields

$$\begin{aligned} |\langle f, \psi_{\ell, k, j} \rangle| &\leq \sqrt{\int_{X_k^\ell} (f(x) - m(f, X_k^\ell))^2 d\nu(x)} \cdot \sqrt{\int_{X_k^\ell} (\psi_{\ell, k, j}(x))^2 d\nu(x)} \\ &= \sigma(f, X_k^\ell). \end{aligned}$$

According to Lemma 2, if f is (C, α) Hölder, it is $(C2^{\alpha+1}, \alpha)$ mean-Hölder. In particular, Eq. (20) implies that

$$|\langle f, \psi_{\ell, k, j} \rangle| \leq C2^{\alpha+1} \cdot \nu(X_k^\ell)^{\alpha+\frac{1}{2}}.$$

□.

Proof of Theorem 2: Let $x, y \in X$ and let κ and λ be such that $folder(x, y) = X_\kappa^\lambda$. Our aim is to show that $|f(x) - f(y)| \leq C' \cdot \nu(X_\kappa^\lambda)^\alpha$ with C' given by Eq. (9).

To this end, we use the decomposition

$$f(x) = \sum_{\ell, k, j} \langle f, \psi_{\ell, k, j} \rangle \psi_{\ell, k, j}(x).$$

Note that by definition, for any coarse level $\ell < \lambda$ the samples x, y belong to the same folders, and thus $\psi_{\ell, k, j}(x) = \psi_{\ell, k, j}(y)$ for any k, j . Hence, the only terms contributing to the difference $f(x) - f(y)$ are those in the finer folders at levels $\ell = \lambda, \dots, L$, where x, y belong to *different* folders. That is,

$$\begin{aligned} f(x) - f(y) &= \sum_{\ell=\lambda}^L \sum_{j \in sub(\ell, \tau(\ell, x))} \langle f, \psi_{\ell, \tau(\ell, x), j} \rangle \cdot \psi_{\ell, \tau(\ell, x), j}(x) \\ &\quad - \sum_{\ell=\lambda}^L \sum_{j \in sub(\ell, \tau(\ell, y))} \langle f, \psi_{\ell, \tau(\ell, y), j} \rangle \cdot \psi_{\ell, \tau(\ell, y), j}(y) \end{aligned}$$

where $\tau(\ell, x)$ is the folder at level ℓ that contains x , $x \in X_{\tau(\ell, x)}^\ell$. Next, recall that by definition the functions $\psi_{\ell, k, j}$ are all normalized, and they are constant on all subfolders of X_k^ℓ . Thus,

$$\|\psi_{\ell, k, j}\|^2 = \sum_{i \in sub(\ell, k)} \nu(X_i^{\ell+1}) \psi_{\ell, k, j}^2(X_i^{\ell+1}) = 1$$

and so

$$|\psi_{\ell, k, j}(x)| \leq \frac{1}{\sqrt{\nu(X_i^{\ell+1})}} \leq \frac{1}{\sqrt{B\nu(X_k^\ell)}}. \quad (21)$$

Combining the bound on $|\psi_{\ell, k, j}|$ with the bound on the coefficient decay of f gives that

$$\begin{aligned} |f(x) - f(y)| &\leq \frac{C}{\sqrt{B}} \sum_{\ell=\lambda}^L \sum_{j \in sub(\ell, \tau(\ell, x))} \nu(X_{\tau(\ell, x)}^\ell)^{\alpha+1/2} \frac{1}{\sqrt{\nu(X_{\tau(\ell, x)}^\ell)}} \\ &\quad + \frac{C}{\sqrt{B}} \sum_{\ell=\lambda}^L \sum_{j \in sub(\ell, \tau(\ell, y))} \nu(X_{\tau(\ell, y)}^\ell)^{\alpha+1/2} \frac{1}{\sqrt{\nu(X_{\tau(\ell, y)}^\ell)}} \end{aligned} \quad (22)$$

Finally, since the tree is balanced, $\nu(X_{\tau(\ell, x)}^\ell) \leq \overline{B}^{\ell-\lambda} \nu(X_\kappa^\lambda)$, and $|sub(\ell, k)| \leq \frac{1}{\overline{B}} - 1$. Thus,

$$\begin{aligned} |f(x) - f(y)| &\leq \frac{2C(1-\overline{B})}{\overline{B}^{3/2}} \sum_{\ell=\lambda}^L \left(\overline{B}^\alpha\right)^{\ell-\lambda} \nu(X_\kappa^\lambda)^\alpha \\ &\leq \frac{2C}{\overline{B}^{3/2}} \frac{1}{1-\overline{B}^\alpha} \nu(X_\kappa^\lambda)^\alpha = C' \nu(X_\kappa^\lambda)^\alpha. \end{aligned}$$

□.

Proof of Theorem 3: Let $\hat{f} = \sum_{|I|>\epsilon} a_I h_I(x)$. Then

$$\begin{aligned} \|f - \hat{f}\|_1 &= \sum_x |f(x) - \hat{f}(x)| = \sum_x \left| \sum_{|I|<\epsilon} a_I h_I(x) \right| \\ &\leq \sum_{|I|<\epsilon} |a_I| \sum_{x \in I} |h_I(x)| \end{aligned} \quad (23)$$

but according to the assumptions of the theorem, $|h_I(x)| \leq 1/|I|^{1/2}$ and $\text{supp}(h_I) = |I|$. Hence, $\sum_{x \in I} |h_I(x)| < \epsilon/\sqrt{\epsilon} = \sqrt{\epsilon}$. Combining this with the entropy condition on the coefficients, $\sum_I |a_I| \leq C$ the theorem follows. \square

Proof of Theorem 4: Recall that the coefficient $\hat{a}_{\ell,k,j}$ is given by Eq. (12) if all subfolders of X_k^ℓ at level $\ell + 1$ each contain at least one labeled point. Otherwise, $\hat{a}_{\ell,k,j}$ is set to zero. Denote by R the event that at least one of the subfolders of X_k^ℓ does not contain labeled points. First of all,

$$\begin{aligned} \Pr[R] &\leq \sum_{i \in \text{sub}(\ell,k)} \Pr[|S \cap X_i^{\ell+1}| = 0] = \sum_{i \in \text{sub}(\ell,k)} (1 - \nu(X_i^{\ell+1}))^{|S|} \\ &\leq \sum_{i \in \text{sub}(\ell,k)} e^{-|S|\nu(X_i^{\ell+1})} \leq \frac{1}{B} e^{-|S|B\nu(X_k^\ell)} \end{aligned}$$

Conditional on the event R , we have $\mathbb{E}[\hat{a}_{\ell,k,j}] = \text{var}[\hat{a}_{\ell,k,j}] = 0$, whereas under R^c , we have that $\mathbb{E}[\hat{a}_{\ell,k,j}] = a_{\ell,k,j}$, and after some algebraic manipulations,

$$\text{var}[\hat{a}_{\ell,k,j} | R^c] = \sum_{i \in \text{sub}(\ell,k)} \nu^2(X_i^{\ell+1}) \psi_{\ell,k,j}^2(X_i^{\ell+1}) \frac{\sigma^2(f, X_i^{\ell+1})}{|S \cap X_i^{\ell+1}|} \quad (24)$$

To compute the mean squared error of the estimator $\hat{a}_{\ell,k,j}$ we use the identity

$$\mathbb{E}[\hat{a}_{\ell,k,j} - a_{\ell,k,j}]^2 = \text{var}[\hat{a}_{\ell,k,j}] + (\mathbb{E}[\hat{a}_{\ell,k,j}] - a_{\ell,k,j})^2. \quad (25)$$

Regarding the second term in (25), we have that $\mathbb{E}[\hat{a}_{\ell,k,j}] = a_{\ell,k,j} (1 - \Pr[R])$. Thus,

$$(\mathbb{E}[\hat{a}_{\ell,k,j}] - a_{\ell,k,j})^2 = a_{\ell,k,j}^2 \Pr[R]^2. \quad (26)$$

As for the first term in (25), let Z be the random variable defined as the indicator function of the event R , $Z = \mathbf{1}_R$. By the variance decomposition formula

$$\text{var}[\hat{a}_{\ell,k,j}] = \mathbb{E}[\text{var}[\hat{a}_{\ell,k,j} | Z]] + \text{var}[\mathbb{E}[\hat{a}_{\ell,k,j} | Z]] \quad (27)$$

Now, by (24),

$$\mathbb{E}[\text{var}[\hat{a}_{\ell,k,j} | Z]] = \Pr[R^c] \sum_{i \in \text{sub}(\ell,k)} \nu^2(X_i^{\ell+1}) \psi_{\ell,k,j}^2(X_i^{\ell+1}) \sigma^2(f, X_i^{\ell+1}) \mathbb{E}\left[\frac{1}{|S \cap X_i^{\ell+1}|} \mid R^c\right]$$

For $|S| \gg 1$, we approximate the conditioning on R^c by the (simpler) conditioning on $\{|S \cap X_i^{\ell+1}| > 0\}$. This gives

$$\mathbb{E}[\text{var}[\hat{a}_{\ell,k,j} | Z]] = \Pr[R^c] \sum_{i \in \text{sub}(\ell,k)} \nu^2(X_i^{\ell+1}) \psi_{\ell,k,j}^2(X_i^{\ell+1}) \sigma^2(f, X_i^{\ell+1}) \frac{\mathbb{E}[A_i]}{\Pr[|S \cap X_i^{\ell+1}| > 0]} \quad (28)$$

where

$$A_i = \begin{cases} \frac{1}{|S \cap X_i^{\ell+1}|} & |S \cap X_i^{\ell+1}| > 0 \\ 0 & |S \cap X_i^{\ell+1}| = 0 \end{cases}.$$

The quantity $\mathbb{E}[A_i]$ is known as the first *inverse moment* of the Binomial distribution $\text{Bin}(|S|, \nu(X_i^{\ell+1}))$. Asymptotic expansions of this quantity have been studied extensively. In Rempala (2003), it was proved that

$$\mathbb{E}[A_i] = \frac{1}{|S| \cdot \nu(X_i^{\ell+1})} + o\left(\frac{1}{|S|}\right).$$

Using this approximation in (28) gives, up to an $o(1/|S|)$ error

$$\mathbb{E}[\text{var}[\hat{a}_{\ell,k,j} | Z]] \approx \frac{\Pr[R^c]}{|S|} \sum_{i \in \text{sub}(\ell,k)} \nu(X_i^{\ell+1}) \psi_{\ell,k,j}^2(X_i^{\ell+1}) \frac{\sigma^2(f, X_i^{\ell+1})}{\Pr[|S \cap X_i^{\ell+1}| > 0]}.$$

As f is (C, α) -Hölder, according to Lemma 2 it is (C_1, α) mean-Hölder with $C_1 = 2^{\alpha+1}C$. Thus, $\sigma^2(f, X_i^{\ell+1}) \leq C_1^2 \nu(X_i^{\ell+1})^{2\alpha}$. Since the tree is balanced, $\nu(X_i^{\ell+1}) \leq \bar{B}\nu(X_k^\ell)$. In addition,

$$\frac{1}{\Pr[|S \cap X_i^{\ell+1}| > 0]} \leq \frac{1}{1 - e^{-|S|\nu(X_i^{\ell+1})}} \leq \frac{1}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}}$$

Therefore,

$$\begin{aligned} \mathbb{E} \left[\text{var} \left[\hat{a}_{\ell,k,j} \middle| Z \right] \right] &\leq \frac{1}{|S|} \frac{C_1^2 \bar{B}^{2\alpha} \nu^{2\alpha}(X_k^\ell)}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}} \sum_{i \in \text{sub}(\ell,k)} \nu(X_i^{\ell+1}) \psi_{\ell,k,j}^2(X_i^{\ell+1}) \\ &= \frac{1}{|S|} \frac{C_1^2 \bar{B}^{2\alpha} \nu^{2\alpha}(X_k^\ell)}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}}. \end{aligned} \quad (29)$$

where the summation is simply $\|\psi_{\ell,k,j}\|^2 = 1$.

For the second term in Eq. (27), note that

$$\mathbb{E} [\hat{a}_{\ell,k,j} | Z] = \begin{cases} a_{\ell,k,j} & \text{under } R^c \\ 0 & \text{under } R \end{cases} \quad (30)$$

Therefore,

$$\text{var} \left[\mathbb{E} \left[\hat{a}_{\ell,k,j} \middle| Z \right] \right] = a_{\ell,k,j}^2 (1 - \Pr[R]) \Pr[R]. \quad (31)$$

Combining (29), (31) into (25) gives that

$$\begin{aligned} \mathbb{E} [\hat{a}_{\ell,k,j} - a_{\ell,k,j}]^2 &\leq \frac{1}{|S|} \frac{C_1^2 \bar{B}^{2\alpha} \nu^{2\alpha}(X_k^\ell)}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}} + a_{\ell,k,j}^2 (1 - \Pr[R]) \Pr[R] + a_{\ell,k,j}^2 \Pr[R]^2 \\ &\leq \frac{1}{|S|} \frac{C_1^2 \bar{B}^{2\alpha} \nu^{2\alpha}(X_k^\ell)}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}} + \frac{1}{\underline{B}} e^{-|S|\underline{B}\nu(X_k^\ell)} \cdot a_{\ell,k,j}^2. \end{aligned} \quad (32)$$

Finally, to prove the formula for the mean squared error in estimating f we note that due to the orthogonality of the Haar-like basis functions,

$$\begin{aligned} \mathbb{E} \left\| f - \hat{f} \right\|^2 &= \mathbb{E} \left[\left\| \sum_{\ell,k,j} (a_{\ell,k,j} - \hat{a}_{\ell,k,j}) \psi_{\ell,k,j} \right\|^2 \right] = \mathbb{E} \left[\sum_{\ell,k,j} (a_{\ell,k,j} - \hat{a}_{\ell,k,j})^2 \right] \\ &= \sum_{\ell,k,j} \mathbb{E} [a_{\ell,k,j} - \hat{a}_{\ell,k,j}]^2. \end{aligned}$$

Hence,

$$\begin{aligned} \mathbb{E} \|f - \hat{f}\|^2 &\leq \frac{C_1^2 \bar{B}^{2\alpha}}{|S|} \sum_{\ell,k,j} \frac{\nu(X_k^\ell)^{2\alpha}}{1 - e^{-|S|\underline{B}\nu(X_k^\ell)}} + \frac{1}{\underline{B}} \sum_{\ell,k,j} e^{-|S|\underline{B}\nu(X_k^\ell)} a_{\ell,k,j}^2 \\ &\leq \frac{C_1^2 \bar{B}^{2\alpha}}{|S|} \sum_{\ell,k,j} \frac{(\bar{B}^{2\alpha})^{\ell-1}}{1 - e^{-|S|\underline{B}^\ell}} + \frac{2^{2\alpha+1} C_1^2}{\underline{B}} \sum_{\ell,k,j} e^{-|S|\underline{B}^\ell} (\bar{B}^{2\alpha+1})^{\ell-1} \end{aligned} \quad (33)$$

□